



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:15 PM EDT

PDB ID : 4M1M / pdb_00004m1m
Title : Corrected Structure of Mouse P-glycoprotein
Authors : Li, J.; Jaimes, K.F.; Aller, S.G.
Deposited on : 2013-08-03
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

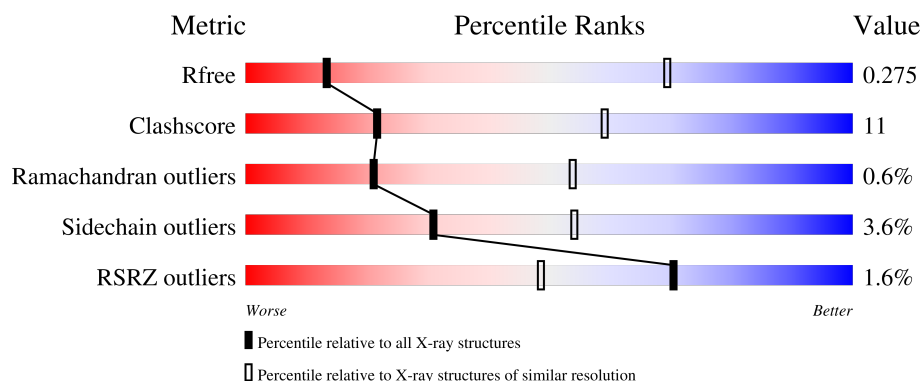
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1282	
1	B	1282	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18378 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1188	Total	C	N	O	S	0	0	0
			9213	5923	1559	1694	37			
1	B	1180	Total	C	N	O	S	0	0	0
			9152	5887	1550	1678	37			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	conflict	UNP P21447
A	87	GLN	ASN	conflict	UNP P21447
A	90	GLN	ASN	conflict	UNP P21447
A	952	ALA	CYS	conflict	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
B	83	GLN	ASN	conflict	UNP P21447
B	87	GLN	ASN	conflict	UNP P21447
B	90	GLN	ASN	conflict	UNP P21447
B	952	ALA	CYS	conflict	UNP P21447
B	1277	HIS	-	expression tag	UNP P21447
B	1278	HIS	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447

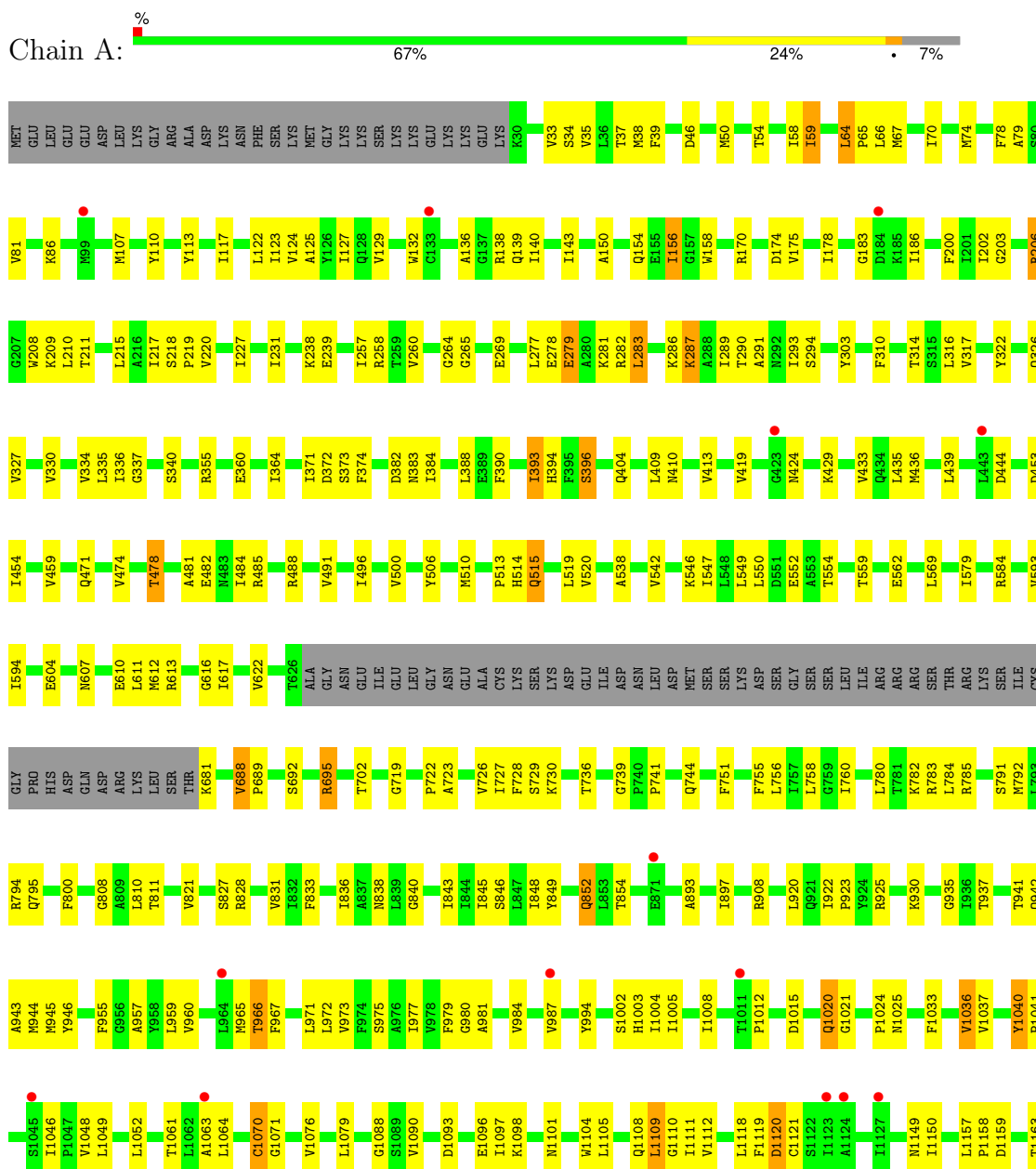
- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

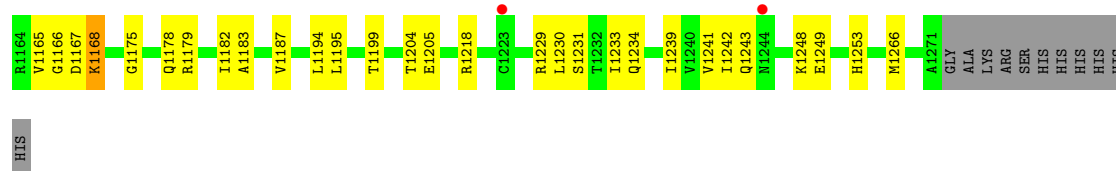
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	Hg 7	0	0
2	B	6	Total 6	Hg 6	0	0

3 Residue-property plots

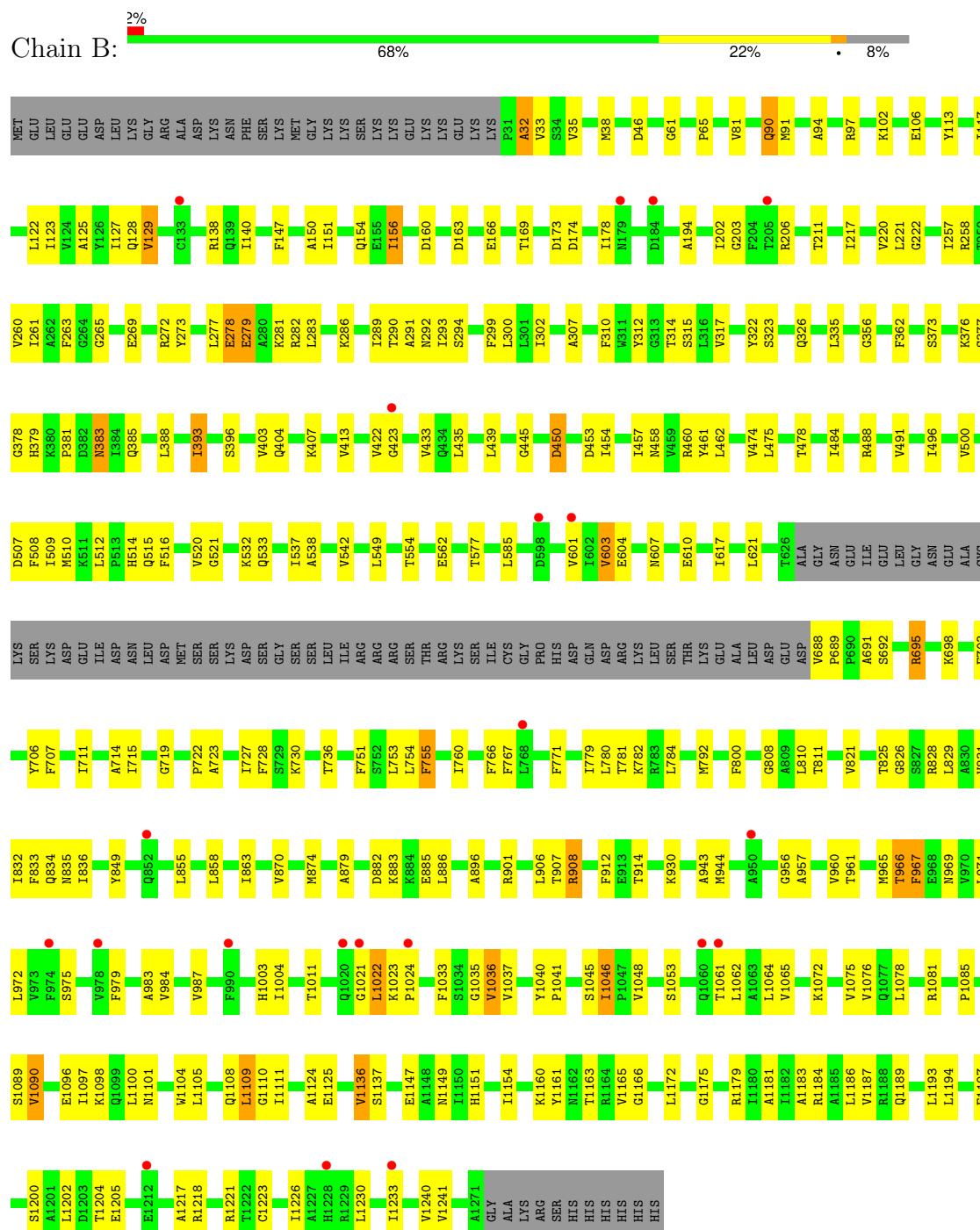
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Multidrug resistance protein 1A





• Molecule 1: Multidrug resistance protein 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.54Å 115.43Å 378.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 3.80 24.89 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.9 (24.89-3.80) 95.5 (24.89-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 3.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.212 , 0.267 0.226 , 0.275	Depositor DCC
R_{free} test set	4245 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	132.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 87.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18378	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/9382	0.84	8/12684 (0.1%)
1	B	0.38	0/9321	0.82	5/12601 (0.0%)
All	All	0.39	0/18703	0.83	13/25285 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	695	ARG	N-CA-C	-7.91	103.08	112.89
1	A	1040	TYR	CA-C-N	6.54	126.23	119.56
1	A	1040	TYR	C-N-CA	6.54	126.23	119.56
1	B	1011	THR	CA-C-N	6.05	126.51	120.52
1	B	1011	THR	C-N-CA	6.05	126.51	120.52
1	A	515	GLN	CB-CA-C	-5.90	109.78	116.63
1	A	1025	ASN	N-CA-C	-5.39	107.25	113.88
1	B	450	ASP	CB-CA-C	-5.26	110.52	116.63
1	A	688	VAL	CA-C-N	-5.24	114.98	120.38
1	A	688	VAL	C-N-CA	-5.24	114.98	120.38
1	B	1036	VAL	N-CA-C	5.12	114.65	107.37
1	A	393	ILE	N-CA-C	5.02	114.50	107.37
1	A	1093	ASP	CB-CA-C	-5.01	110.81	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9213	0	9383	218	0
1	B	9152	0	9333	186	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
All	All	18378	0	18716	401	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HZ2	1:A:782:LYS:HA	1.28	0.97
1:A:559:THR:HG22	1:A:584:ARG:HH12	1.39	0.87
1:B:1021:GLY:HA2	1:B:1101:ASN:HB2	1.60	0.81
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.64	0.80
1:A:1149:ASN:O	1:A:1179:ARG:NH2	2.14	0.79
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.64	0.79
1:B:257:ILE:HG12	1:B:800:PHE:CE2	2.20	0.77
1:A:966:THR:OG1	1:A:967:PHE:N	2.15	0.77
1:B:1022:LEU:HD11	1:B:1100:LEU:HA	1.67	0.75
1:A:257:ILE:HG12	1:A:800:PHE:CE2	2.22	0.75
1:A:396:SER:HB3	1:A:404:GLN:HA	1.70	0.72
1:B:784:LEU:HD22	1:B:821:VAL:HG11	1.72	0.72
1:A:281:LYS:NZ	1:A:785:ARG:HD2	2.05	0.71
1:A:122:LEU:HB3	1:A:943:ALA:HB2	1.72	0.71
1:B:257:ILE:HG12	1:B:800:PHE:HE2	1.54	0.70
1:A:281:LYS:NZ	1:A:782:LYS:HA	2.06	0.70
1:A:208:TRP:HE3	1:A:209:LYS:HG2	1.55	0.70
1:A:281:LYS:HZ3	1:A:785:ARG:HD2	1.58	0.69
1:A:854:THR:HG23	1:A:977:ILE:HD11	1.74	0.69
1:A:208:TRP:CE3	1:A:209:LYS:HG2	2.28	0.69
1:A:239:GLU:OE1	1:A:287:LYS:NZ	2.20	0.68
1:A:257:ILE:HG12	1:A:800:PHE:HE2	1.57	0.68
1:B:272:ARG:NH2	1:B:1125:GLU:OE2	2.27	0.68
1:B:966:THR:H	1:B:967:PHE:HA	1.59	0.67
1:A:59:ILE:HD11	1:A:124:VAL:HG11	1.76	0.66
1:A:384:ILE:HD11	1:A:546:LYS:HB2	1.78	0.66
1:B:484:ILE:HG21	1:B:496:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASP:OD1	1:B:901:ARG:NH2	2.29	0.66
1:B:396:SER:OG	1:B:403:VAL:O	2.14	0.65
1:A:34:SER:OG	1:A:37:THR:OG1	2.13	0.65
1:B:94:ALA:HB1	1:B:97:ARG:HE	1.62	0.64
1:B:122:LEU:HB3	1:B:943:ALA:HB2	1.78	0.63
1:A:388:LEU:HB2	1:A:413:VAL:HB	1.81	0.63
1:B:282:ARG:HH22	1:B:779:ILE:HA	1.65	0.62
1:A:371:ILE:O	1:A:373:SER:HB3	2.00	0.62
1:A:206:ARG:HE	1:A:206:ARG:HA	1.65	0.61
1:A:794:ARG:HG2	1:A:1012:PRO:HG3	1.82	0.61
1:B:102:LYS:HE3	1:B:106:GLU:OE2	2.00	0.61
1:A:780:LEU:O	1:A:784:LEU:HB2	1.99	0.61
1:A:513:PRO:HB2	1:A:514:HIS:CD2	2.35	0.61
1:A:70:ILE:HD13	1:A:113:TYR:HB3	1.82	0.60
1:B:1033:PHE:HD1	1:B:1036:VAL:HG21	1.67	0.59
1:A:419:VAL:HG22	1:A:593:VAL:HB	1.85	0.59
1:A:784:LEU:HD22	1:A:821:VAL:HG11	1.84	0.59
1:A:1112:VAL:HB	1:A:1195:LEU:HD23	1.84	0.59
1:A:554:THR:HB	1:A:562:GLU:HG3	1.84	0.58
1:A:337:GLY:O	1:A:340:SER:OG	2.21	0.58
1:A:833:PHE:HA	1:A:836:ILE:HG22	1.84	0.58
1:A:1110:GLY:O	1:A:1194:LEU:N	2.33	0.58
1:A:840:GLY:O	1:A:843:ILE:HG22	2.04	0.57
1:A:1199:THR:OG1	1:A:1229:ARG:NH2	2.37	0.57
1:A:1036:VAL:H	1:A:1088:GLY:HA3	1.70	0.57
1:B:378:GLY:H	1:B:458:ASN:HB2	1.69	0.57
1:A:1021:GLY:HA3	1:A:1101:ASN:HB2	1.88	0.56
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.38	0.56
1:B:1149:ASN:O	1:B:1179:ARG:NH2	2.38	0.56
1:B:65:PRO:HB2	1:B:202:ILE:HD12	1.87	0.56
1:A:510:MET:SD	1:A:515:GLN:NE2	2.79	0.56
1:B:1096:GLU:OE1	1:B:1098:LYS:N	2.32	0.56
1:B:1065:VAL:HG23	1:B:1241:VAL:HA	1.87	0.56
1:A:123:ILE:O	1:A:127:ILE:HG12	2.05	0.56
1:A:792:MET:HE1	1:A:810:LEU:HB3	1.88	0.56
1:B:1072:LYS:HD3	1:B:1226:ILE:HG23	1.88	0.56
1:A:1079:LEU:HG	1:A:1109:LEU:HD21	1.89	0.55
1:A:215:LEU:O	1:A:218:SER:OG	2.23	0.55
1:B:510:MET:SD	1:B:515:GLN:NE2	2.80	0.55
1:A:1096:GLU:OE1	1:A:1098:LYS:N	2.36	0.55
1:A:310:PHE:CD2	1:A:755:PHE:HE2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ALA:H	1:B:356:GLY:HA2	1.71	0.55
1:A:893:ALA:O	1:A:897:ILE:HG12	2.06	0.55
1:B:289:ILE:HD13	1:B:771:PHE:HE1	1.72	0.55
1:B:291:ALA:O	1:B:294:SER:OG	2.22	0.54
1:B:292:ASN:ND2	1:B:766:PHE:O	2.41	0.54
1:A:200:PHE:HE2	1:A:215:LEU:HD12	1.72	0.54
1:B:457:ILE:HD11	1:B:462:LEU:HD13	1.88	0.54
1:A:612:MET:HE1	1:A:622:VAL:HG21	1.89	0.54
1:B:554:THR:HB	1:B:562:GLU:HG3	1.89	0.54
1:A:281:LYS:HZ2	1:A:782:LYS:CA	2.12	0.54
1:B:500:VAL:HG11	1:B:509:ILE:HD12	1.90	0.54
1:A:453:ASP:OD1	1:A:454:ILE:N	2.41	0.53
1:B:393:ILE:H	1:B:445:GLY:HA3	1.73	0.53
1:A:846:SER:HB2	1:A:973:VAL:HG13	1.90	0.53
1:A:1230:LEU:HD23	1:A:1233:ILE:HD12	1.89	0.53
1:B:206:ARG:O	1:B:326:GLN:NE2	2.36	0.53
1:B:475:LEU:HD12	1:B:532:LYS:HG2	1.90	0.53
1:A:373:SER:HB2	1:A:459:VAL:HG11	1.90	0.53
1:B:289:ILE:O	1:B:293:ILE:HG12	2.08	0.53
1:B:1033:PHE:CD1	1:B:1036:VAL:HG21	2.43	0.53
1:A:393:ILE:HB	1:A:409:LEU:HB3	1.89	0.53
1:A:485:ARG:NH2	1:B:914:THR:OG1	2.42	0.53
1:A:175:VAL:HA	1:A:178:ILE:HG22	1.91	0.53
1:B:206:ARG:HG3	1:B:326:GLN:HG3	1.90	0.53
1:A:66:LEU:HD23	1:A:202:ILE:HD11	1.90	0.53
1:A:1020:GLN:HG2	1:A:1021:GLY:N	2.23	0.53
1:A:1049:LEU:HD13	1:A:1052:LEU:HD21	1.91	0.53
1:A:496:ILE:O	1:A:500:VAL:HG23	2.09	0.53
1:A:1234:GLN:HG2	1:A:1253:HIS:CE1	2.44	0.53
1:A:607:ASN:HB3	1:A:610:GLU:OE2	2.08	0.52
1:B:711:ILE:O	1:B:715:ILE:HG13	2.09	0.52
1:B:277:LEU:C	1:B:279:GLU:H	2.17	0.52
1:B:907:THR:O	1:B:908:ARG:NE	2.42	0.52
1:B:1136:VAL:HG22	1:B:1137:SER:H	1.75	0.52
1:A:316:LEU:HD23	1:A:322:TYR:CD1	2.44	0.52
1:A:728:PHE:CE1	1:A:971:LEU:HD21	2.44	0.52
1:B:695:ARG:HA	1:B:698:LYS:NZ	2.25	0.52
1:B:835:ASN:CG	1:B:984:VAL:HG13	2.35	0.52
1:A:506:TYR:OH	1:A:510:MET:HE3	2.10	0.52
1:A:925:ARG:HA	1:B:514:HIS:HD2	1.74	0.52
1:A:46:ASP:OD1	1:A:138:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLU:O	1:A:364:ILE:HG12	2.10	0.51
1:A:1120:ASP:HB3	1:A:1168:LYS:HD3	1.92	0.51
1:A:33:VAL:HG12	1:A:37:THR:HB	1.91	0.51
1:B:460:ARG:HG3	1:B:907:THR:HG21	1.92	0.51
1:B:300:LEU:HD11	1:B:760:ILE:HD13	1.92	0.51
1:B:317:VAL:HG23	1:B:323:SER:HA	1.92	0.51
1:B:507:ASP:OD1	1:B:508:PHE:N	2.44	0.51
1:B:520:VAL:HG22	1:B:521:GLY:H	1.75	0.51
1:A:831:VAL:HG13	1:A:987:VAL:HG12	1.93	0.51
1:A:937:THR:O	1:A:941:THR:HG23	2.11	0.51
1:A:1104:TRP:NE1	1:A:1108:GLN:HE22	2.09	0.51
1:B:965:MET:HB3	1:B:966:THR:OG1	2.11	0.51
1:B:1230:LEU:HD23	1:B:1233:ILE:HD12	1.92	0.51
1:A:1033:PHE:HD1	1:A:1036:VAL:HG11	1.76	0.51
1:B:792:MET:HE1	1:B:810:LEU:HB3	1.93	0.51
1:A:170:ARG:HG3	1:A:174:ASP:HB2	1.93	0.50
1:A:175:VAL:O	1:A:178:ILE:HG22	2.11	0.50
1:A:382:ASP:OD1	1:A:382:ASP:N	2.43	0.50
1:B:723:ALA:O	1:B:727:ILE:HG12	2.10	0.50
1:B:496:ILE:O	1:B:500:VAL:HG23	2.11	0.50
1:B:849:TYR:HB3	1:B:969:ASN:HB3	1.92	0.50
1:B:1097:ILE:HG23	1:B:1105:LEU:HD22	1.92	0.50
1:A:756:LEU:O	1:A:760:ILE:HG12	2.12	0.50
1:B:379:HIS:H	1:B:457:ILE:HA	1.77	0.50
1:A:34:SER:HG	1:A:37:THR:HG1	1.53	0.50
1:B:94:ALA:HB1	1:B:97:ARG:NE	2.27	0.50
1:A:238:LYS:HG2	1:A:283:LEU:HD11	1.93	0.49
1:A:612:MET:HE1	1:A:622:VAL:HG11	1.94	0.49
1:B:1110:GLY:HA3	1:B:1193:LEU:HD23	1.94	0.49
1:A:538:ALA:O	1:A:542:VAL:HG23	2.12	0.49
1:A:1150:ILE:HG22	1:A:1179:ARG:HB3	1.94	0.49
1:B:808:GLY:HA2	1:B:811:THR:HG22	1.94	0.49
1:A:723:ALA:O	1:A:727:ILE:HG12	2.13	0.49
1:A:852:GLN:CD	1:A:852:GLN:H	2.20	0.49
1:A:1241:VAL:HB	1:A:1249:GLU:HB2	1.93	0.49
1:B:312:TYR:O	1:B:315:SER:OG	2.21	0.49
1:B:381:PRO:O	1:B:461:TYR:OH	2.24	0.49
1:A:260:VAL:O	1:A:264:GLY:N	2.45	0.49
1:A:424:ASN:H	1:A:429:LYS:HZ1	1.60	0.49
1:B:281:LYS:HD2	1:B:781:THR:HB	1.92	0.49
1:B:879:ALA:O	1:B:883:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:HIS:HB2	1:A:444:ASP:HB3	1.94	0.49
1:A:227:ILE:O	1:A:231:ILE:HG13	2.13	0.49
1:A:604:GLU:OE2	1:A:616:GLY:HA3	2.12	0.49
1:A:981:ALA:O	1:A:984:VAL:HG22	2.13	0.49
1:B:784:LEU:HD21	1:B:1004:ILE:HG21	1.95	0.49
1:A:617:ILE:HD12	1:A:617:ILE:H	1.77	0.48
1:A:794:ARG:NH1	1:A:1015:ASP:OD2	2.46	0.48
1:A:920:LEU:O	1:A:923:PRO:HD2	2.13	0.48
1:A:79:ALA:HB2	1:A:736:THR:HG22	1.95	0.48
1:B:278:GLU:HG3	1:B:282:ARG:HD2	1.95	0.48
1:B:257:ILE:HD12	1:B:260:VAL:HB	1.95	0.48
1:A:388:LEU:HD11	1:A:547:ILE:HD13	1.95	0.48
1:B:966:THR:OG1	1:B:969:ASN:HB2	2.14	0.48
1:B:1078:LEU:HD22	1:B:1085:PRO:HD3	1.95	0.48
1:B:388:LEU:HD13	1:B:577:THR:HG21	1.96	0.48
1:A:1178:GLN:O	1:A:1182:ILE:HG12	2.13	0.48
1:B:61:GLY:HA3	1:B:194:ALA:HB3	1.96	0.48
1:B:870:VAL:HG12	1:B:874:MET:HE2	1.96	0.48
1:B:299:PHE:HA	1:B:302:ILE:HG12	1.95	0.48
1:B:1022:LEU:HD11	1:B:1100:LEU:HD23	1.95	0.48
1:A:277:LEU:C	1:A:279:GLU:H	2.22	0.48
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.96	0.48
1:B:1061:THR:HG21	1:B:1218:ARG:HD3	1.95	0.48
1:B:217:ILE:O	1:B:220:VAL:HG12	2.13	0.47
1:B:453:ASP:OD1	1:B:454:ILE:N	2.47	0.47
1:B:1045:SER:OG	1:B:1046:ILE:N	2.47	0.47
1:A:158:TRP:HZ2	1:A:364:ILE:HD12	1.79	0.47
1:B:90:GLN:HG2	1:B:91:MET:H	1.79	0.47
1:B:855:LEU:HA	1:B:858:LEU:HG	1.95	0.47
1:B:385:GLN:HB2	1:B:450:ASP:OD2	2.13	0.47
1:A:1158:PRO:HA	1:A:1159:ASP:HA	1.62	0.47
1:B:960:VAL:HG21	1:B:967:PHE:HB2	1.96	0.47
1:B:1035:GLY:N	1:B:1053:SER:OG	2.40	0.47
1:B:1204:THR:OG1	1:B:1205:GLU:N	2.43	0.47
1:B:533:GLN:O	1:B:537:ILE:HG13	2.13	0.47
1:B:1175:GLY:HA2	1:B:1202:LEU:HD11	1.95	0.47
1:B:585:LEU:HD11	1:B:621:LEU:HB3	1.97	0.47
1:B:376:LYS:HA	1:B:377:SER:HA	1.63	0.47
1:A:129:VAL:HG13	1:A:935:GLY:HA2	1.97	0.47
1:B:174:ASP:O	1:B:178:ILE:HG13	2.14	0.47
1:B:689:PRO:HG3	1:B:1003:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:LEU:O	1:B:784:LEU:HB2	2.15	0.47
1:A:86:LYS:HZ2	1:A:739:GLY:HA2	1.80	0.46
1:B:714:ALA:HB1	1:B:834:GLN:HG3	1.97	0.46
1:B:1183:ALA:O	1:B:1187:VAL:HG23	2.15	0.46
1:A:562:GLU:OE1	1:A:584:ARG:NH1	2.48	0.46
1:A:702:THR:OG1	1:A:783:ARG:NH2	2.48	0.46
1:A:1024:PRO:HD2	1:A:1104:TRP:CZ2	2.51	0.46
1:B:538:ALA:O	1:B:542:VAL:HG23	2.15	0.46
1:B:122:LEU:HD12	1:B:123:ILE:N	2.30	0.46
1:B:263:PHE:CZ	1:B:1184:ARG:HD3	2.51	0.46
1:A:481:ALA:O	1:A:485:ARG:HG2	2.16	0.46
1:A:488:ARG:HA	1:A:908:ARG:HH11	1.80	0.46
1:B:140:ILE:HD13	1:B:140:ILE:HA	1.84	0.46
1:B:163:ASP:HB3	1:B:166:GLU:HG2	1.97	0.46
1:A:719:GLY:C	1:A:722:PRO:HD2	2.40	0.46
1:B:125:ALA:O	1:B:129:VAL:HG12	2.16	0.46
1:A:730:LYS:HB3	1:A:751:PHE:CE2	2.50	0.46
1:A:1183:ALA:O	1:A:1187:VAL:HG23	2.15	0.46
1:A:64:LEU:HD12	1:A:336:ILE:HG21	1.98	0.45
1:A:203:GLY:C	1:A:211:THR:HG21	2.41	0.45
1:A:1159:ASP:OD1	1:A:1159:ASP:N	2.43	0.45
1:A:265:GLY:O	1:A:269:GLU:HG2	2.16	0.45
1:A:957:ALA:HA	1:A:960:VAL:HG12	1.97	0.45
1:B:727:ILE:HD12	1:B:754:LEU:HD23	1.98	0.45
1:B:736:THR:HG21	1:B:967:PHE:HE2	1.80	0.45
1:A:314:THR:HA	1:A:317:VAL:HG12	1.97	0.45
1:A:827:SER:O	1:A:831:VAL:HG23	2.17	0.45
1:B:1151:HIS:ND1	1:B:1154:ILE:HD11	2.31	0.45
1:B:1165:VAL:HA	1:B:1166:GLY:HA2	1.79	0.45
1:A:74:MET:HG3	1:A:107:MET:HE1	1.98	0.45
1:B:728:PHE:CE2	1:B:971:LEU:HD21	2.52	0.45
1:A:286:LYS:O	1:A:290:THR:HG23	2.16	0.45
1:A:792:MET:HE3	1:A:810:LEU:HD22	1.99	0.45
1:A:257:ILE:HD12	1:A:260:VAL:HB	1.99	0.45
1:A:471:GLN:HB3	1:A:552:GLU:HB2	1.98	0.45
1:A:478:THR:HB	1:A:482:GLU:HB2	1.98	0.45
1:B:307:ALA:HA	1:B:755:PHE:CE1	2.51	0.45
1:B:38:MET:HA	1:B:362:PHE:HE2	1.81	0.45
1:B:404:GLN:HB3	1:B:407:LYS:NZ	2.32	0.45
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	1.98	0.45
1:A:217:ILE:O	1:A:220:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:VAL:HG21	1:B:516:PHE:HE1	1.82	0.45
1:B:607:ASN:HB3	1:B:610:GLU:OE1	2.16	0.45
1:B:908:ARG:HE	1:B:908:ARG:HA	1.83	0.44
1:A:1061:THR:HG21	1:A:1218:ARG:HD3	1.98	0.44
1:A:784:LEU:HD21	1:A:1004:ILE:HG21	1.99	0.44
1:B:617:ILE:HD12	1:B:617:ILE:H	1.82	0.44
1:A:689:PRO:HG3	1:A:1003:HIS:CD2	2.52	0.44
1:A:741:PRO:HA	1:A:744:GLN:HG3	1.98	0.44
1:A:945:MET:HB2	1:A:945:MET:HE3	1.67	0.44
1:A:1165:VAL:HA	1:A:1166:GLY:HA2	1.71	0.44
1:B:407:LYS:O	1:B:601:VAL:HG22	2.17	0.44
1:B:882:ASP:HA	1:B:885:GLU:HG2	2.00	0.44
1:A:38:MET:SD	1:A:355:ARG:HG2	2.58	0.44
1:A:65:PRO:HB2	1:A:202:ILE:HD12	1.99	0.44
1:A:975:SER:O	1:A:979:PHE:HB2	2.18	0.44
1:B:265:GLY:O	1:B:269:GLU:HG2	2.18	0.44
1:A:1119:PHE:C	1:A:1121:CYS:H	2.25	0.44
1:B:1081:ARG:HD3	1:B:1097:ILE:CG2	2.47	0.44
1:A:78:PHE:CZ	1:A:107:MET:HE3	2.52	0.44
1:A:610:GLU:HG3	1:A:613:ARG:HH21	1.83	0.44
1:B:65:PRO:CB	1:B:202:ILE:HD12	2.48	0.44
1:B:273:TYR:CE2	1:B:277:LEU:HD11	2.53	0.44
1:B:283:LEU:HD23	1:B:286:LYS:HD2	2.00	0.44
1:B:1108:GLN:O	1:B:1109:LEU:HD12	2.18	0.44
1:B:692:SER:OG	1:B:695:ARG:HB3	2.18	0.44
1:A:150:ALA:O	1:A:154:GLN:HG2	2.17	0.43
1:A:326:GLN:O	1:A:330:VAL:HG22	2.18	0.43
1:A:692:SER:OG	1:A:695:ARG:HB3	2.18	0.43
1:A:1079:LEU:HD23	1:A:1194:LEU:HD21	2.01	0.43
1:A:1097:ILE:HG23	1:A:1105:LEU:HD22	2.00	0.43
1:A:50:MET:HE1	1:A:139:GLN:HE22	1.83	0.43
1:A:125:ALA:O	1:A:129:VAL:HG12	2.18	0.43
1:A:808:GLY:HA2	1:A:811:THR:HG22	1.99	0.43
1:B:113:TYR:O	1:B:117:ILE:HG13	2.18	0.43
1:B:1104:TRP:NE1	1:B:1108:GLN:HE22	2.16	0.43
1:B:1124:ALA:HB2	1:B:1161:TYR:HB2	2.00	0.43
1:A:925:ARG:HG3	1:B:514:HIS:CD2	2.53	0.43
1:B:957:ALA:O	1:B:961:THR:HG23	2.18	0.43
1:B:975:SER:O	1:B:979:PHE:HB2	2.18	0.43
1:B:1040:TYR:HA	1:B:1041:PRO:HD3	1.90	0.43
1:A:289:ILE:O	1:A:293:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1197:GLU:HB3	1:B:1200:SER:HB3	2.00	0.43
1:A:215:LEU:O	1:A:219:PRO:HD3	2.18	0.43
1:A:726:VAL:O	1:A:730:LYS:HG2	2.18	0.43
1:A:1036:VAL:N	1:A:1088:GLY:HA3	2.31	0.43
1:B:293:ILE:HD12	1:B:767:PHE:HD1	1.83	0.43
1:B:488:ARG:CZ	1:B:491:VAL:HG12	2.49	0.43
1:A:210:LEU:HD21	1:A:327:VAL:HG13	2.01	0.43
1:A:371:ILE:C	1:A:373:SER:HB3	2.44	0.43
1:A:491:VAL:HG11	1:A:542:VAL:CG1	2.48	0.43
1:B:488:ARG:HB3	1:B:491:VAL:HG13	2.00	0.43
1:A:122:LEU:HD12	1:A:123:ILE:N	2.34	0.43
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.86	0.43
1:A:1002:SER:HA	1:A:1005:ILE:HG12	2.01	0.43
1:B:422:VAL:HG22	1:B:423:GLY:H	1.83	0.43
1:B:1062:LEU:HD11	1:B:1240:VAL:HG23	2.01	0.43
1:A:488:ARG:NH2	1:A:491:VAL:HG12	2.34	0.43
1:B:156:ILE:HD11	1:B:439:LEU:O	2.17	0.43
1:B:281:LYS:HG3	1:B:782:LYS:HB2	2.01	0.43
1:B:707:PHE:O	1:B:711:ILE:HG13	2.19	0.43
1:B:896:ALA:HB2	1:B:912:PHE:CD2	2.54	0.43
1:B:1022:LEU:O	1:B:1024:PRO:HD3	2.19	0.43
1:B:1061:THR:HG22	1:B:1223:CYS:HB3	2.00	0.43
1:A:211:THR:HG22	1:A:334:VAL:HG21	2.00	0.43
1:A:727:ILE:HB	1:A:755:PHE:HE1	1.84	0.43
1:A:1118:LEU:HD12	1:A:1165:VAL:HG11	2.01	0.43
1:B:691:ALA:HB1	1:B:692:SER:HA	2.01	0.43
1:A:86:LYS:NZ	1:A:739:GLY:HA2	2.33	0.42
1:A:784:LEU:CD2	1:A:821:VAL:HG11	2.48	0.42
1:A:1266:MET:HE2	1:A:1266:MET:HB3	1.87	0.42
1:B:488:ARG:NH2	1:B:491:VAL:HG12	2.34	0.42
1:B:1033:PHE:CE2	1:B:1075:VAL:HG13	2.54	0.42
1:B:1081:ARG:HD3	1:B:1097:ILE:HG22	2.01	0.42
1:A:54:THR:CG2	1:A:132:TRP:HZ2	2.32	0.42
1:B:46:ASP:CG	1:B:138:ARG:HH12	2.28	0.42
1:B:828:ARG:HA	1:B:831:VAL:HG22	1.99	0.42
1:A:848:ILE:HG13	1:A:849:TYR:CD1	2.53	0.42
1:B:730:LYS:HB3	1:B:751:PHE:CE2	2.54	0.42
1:B:792:MET:CE	1:B:810:LEU:HB3	2.49	0.42
1:B:1064:LEU:HB2	1:B:1226:ILE:HG13	2.01	0.42
1:A:303:TYR:HE1	1:A:758:LEU:HD23	1.84	0.42
1:A:980:GLY:O	1:A:984:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:CYS:HA	1:A:1071:GLY:HA2	1.56	0.42
1:B:169:THR:O	1:B:173:ASP:HB2	2.19	0.42
1:B:603:VAL:HG13	1:B:604:GLU:H	1.84	0.42
1:A:132:TRP:CZ3	1:A:186:ILE:HD11	2.55	0.42
1:A:372:ASP:HA	1:A:373:SER:HB3	2.01	0.42
1:A:424:ASN:H	1:A:429:LYS:NZ	2.17	0.42
1:A:436:MET:HB3	1:A:549:LEU:HD21	2.02	0.42
1:B:123:ILE:O	1:B:127:ILE:HG12	2.19	0.42
1:B:221:LEU:HD12	1:B:222:GLY:N	2.35	0.42
1:B:1147:GLU:CD	1:B:1186:LEU:HD21	2.43	0.42
1:A:156:ILE:HD11	1:A:439:LEU:C	2.44	0.42
1:A:604:GLU:OE1	1:A:617:ILE:N	2.52	0.42
1:A:1064:LEU:HD22	1:A:1242:ILE:HD11	2.00	0.42
1:A:482:GLU:HA	1:A:485:ARG:HG2	2.01	0.42
1:A:944:MET:HE2	1:A:944:MET:HB3	1.78	0.42
1:B:286:LYS:O	1:B:290:THR:HG23	2.20	0.42
1:B:1181:ALA:O	1:B:1184:ARG:HB3	2.20	0.42
1:B:610:GLU:OE1	1:B:610:GLU:N	2.52	0.42
1:A:1040:TYR:HA	1:A:1041:PRO:HD3	1.73	0.42
1:B:257:ILE:HG13	1:B:261:ILE:HG13	2.02	0.42
1:B:1160:LYS:HB3	1:B:1161:TYR:H	1.65	0.42
1:A:922:ILE:HB	1:A:923:PRO:HD3	2.01	0.42
1:B:703:GLU:HB3	1:B:706:TYR:HD2	1.84	0.42
1:A:46:ASP:CG	1:A:138:ARG:HH12	2.26	0.41
1:A:282:ARG:HE	1:A:282:ARG:N	2.17	0.41
1:A:484:ILE:HG21	1:A:496:ILE:HG23	2.01	0.41
1:B:508:PHE:O	1:B:512:LEU:HG	2.20	0.41
1:A:335:LEU:HD12	1:A:335:LEU:HA	1.87	0.41
1:A:156:ILE:HD11	1:A:439:LEU:O	2.19	0.41
1:A:200:PHE:CE2	1:A:215:LEU:HD12	2.54	0.41
1:A:390:PHE:O	1:A:410:ASN:HA	2.19	0.41
1:B:46:ASP:OD1	1:B:138:ARG:NH1	2.54	0.41
1:B:289:ILE:HD13	1:B:771:PHE:CE1	2.54	0.41
1:A:39:PHE:CD1	1:A:50:MET:HE1	2.55	0.41
1:A:67:MET:HE3	1:A:946:TYR:CD2	2.55	0.41
1:A:484:ILE:HG23	1:A:542:VAL:HG21	2.03	0.41
1:A:54:THR:HG23	1:A:132:TRP:HZ2	1.85	0.41
1:A:136:ALA:HB2	1:A:183:GLY:HA2	2.02	0.41
1:A:291:ALA:O	1:A:294:SER:OG	2.27	0.41
1:B:404:GLN:HB3	1:B:407:LYS:HZ3	1.86	0.41
1:B:1100:LEU:HD13	1:B:1105:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:O	1:A:58:ILE:HG12	2.21	0.41
1:A:594:ILE:HB	1:A:611:LEU:HD22	2.02	0.41
1:A:1049:LEU:HD21	1:A:1071:GLY:HA3	2.02	0.41
1:A:1076:VAL:HG13	1:A:1194:LEU:HB3	2.02	0.41
1:A:1157:LEU:HD12	1:A:1158:PRO:HD2	2.03	0.41
1:B:322:TYR:O	1:B:326:GLN:HB3	2.21	0.41
1:A:113:TYR:O	1:A:117:ILE:HG13	2.21	0.41
1:B:150:ALA:O	1:B:154:GLN:HG2	2.20	0.41
1:B:1023:LYS:HA	1:B:1024:PRO:HD3	1.82	0.41
1:B:1089:SER:HB3	1:B:1096:GLU:HG2	2.03	0.41
1:B:1217:ALA:O	1:B:1221:ARG:HD2	2.20	0.41
1:A:64:LEU:HB3	1:A:65:PRO:HD3	2.02	0.41
1:A:550:LEU:HD23	1:A:569:LEU:HD13	2.02	0.41
1:B:257:ILE:HG21	1:B:800:PHE:CD2	2.55	0.41
1:B:388:LEU:HB2	1:B:413:VAL:HB	2.02	0.41
1:A:828:ARG:HA	1:A:828:ARG:HD2	1.88	0.41
1:A:955:PHE:O	1:A:959:LEU:HG	2.20	0.41
1:A:1004:ILE:O	1:A:1008:ILE:HG13	2.20	0.41
1:A:1229:ARG:C	1:A:1231:SER:H	2.28	0.41
1:B:719:GLY:C	1:B:722:PRO:HD2	2.45	0.41
1:B:825:THR:OG1	1:B:826:GLY:N	2.53	0.41
1:B:833:PHE:HD1	1:B:836:ILE:HD11	1.86	0.41
1:A:519:LEU:HD22	1:A:519:LEU:H	1.85	0.41
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	2.02	0.41
1:B:156:ILE:H	1:B:156:ILE:HG13	1.59	0.41
1:B:314:THR:HA	1:B:317:VAL:HG12	2.02	0.41
1:B:956:GLY:O	1:B:960:VAL:HG23	2.21	0.41
1:A:1243:GLN:OE1	1:A:1248:LYS:HD2	2.20	0.40
1:B:983:ALA:O	1:B:987:VAL:HG23	2.22	0.40
1:A:140:ILE:HD13	1:A:140:ILE:HA	1.85	0.40
1:A:156:ILE:HG12	1:A:439:LEU:HB3	2.03	0.40
1:A:310:PHE:HD2	1:A:755:PHE:HE2	1.63	0.40
1:A:828:ARG:HG2	1:A:994:TYR:CE2	2.55	0.40
1:A:845:ILE:HG22	1:A:972:LEU:HD21	2.03	0.40
1:B:147:PHE:O	1:B:151:ILE:HG13	2.21	0.40
1:A:729:SER:OG	1:A:972:LEU:HD12	2.21	0.40
1:A:791:SER:O	1:A:795:GLN:HG2	2.20	0.40
1:A:1175:GLY:O	1:A:1179:ARG:HG3	2.22	0.40
1:B:1090:VAL:O	1:B:1097:ILE:HG13	2.20	0.40
1:B:1096:GLU:OE1	1:B:1097:ILE:N	2.54	0.40
1:A:107:MET:SD	1:A:110:TYR:HD2	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:O	1:A:143:ILE:HG13	2.22	0.40
1:B:203:GLY:C	1:B:211:THR:HG21	2.46	0.40
1:B:1189:GLN:OE1	1:B:1221:ARG:NH2	2.55	0.40
1:B:728:PHE:HE2	1:B:971:LEU:HD21	1.87	0.40
1:B:829:LEU:O	1:B:832:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1184/1282 (92%)	1124 (95%)	54 (5%)	6 (0%)	24	57
1	B	1176/1282 (92%)	1111 (94%)	57 (5%)	8 (1%)	18	51
All	All	2360/2564 (92%)	2235 (95%)	111 (5%)	14 (1%)	21	54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1036	VAL
1	B	32	ALA
1	B	1136	VAL
1	A	1070	CYS
1	A	1120	ASP
1	B	393	ILE
1	A	278	GLU
1	A	838	ASN
1	B	278	GLU
1	B	383	ASN
1	B	1172	LEU
1	B	128	GLN
1	B	33	VAL

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Mol	Chain	Res	Type
1	A	1046	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	978/1062 (92%)	943 (96%)	35 (4%)	31	54
1	B	972/1062 (92%)	937 (96%)	35 (4%)	31	54
All	All	1950/2124 (92%)	1880 (96%)	70 (4%)	31	54

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	59	ILE
1	A	64	LEU
1	A	81	VAL
1	A	156	ILE
1	A	206	ARG
1	A	258	ARG
1	A	279	GLU
1	A	283	LEU
1	A	287	LYS
1	A	374	PHE
1	A	383	ASN
1	A	396	SER
1	A	435	LEU
1	A	474	VAL
1	A	478	THR
1	A	520	VAL
1	A	579	ILE
1	A	681	LYS
1	A	688	VAL
1	A	695	ARG
1	A	852	GLN

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Mol	Chain	Res	Type
1	A	930	LYS
1	A	942	GLN
1	A	965	MET
1	A	966	THR
1	A	1020	GLN
1	A	1037	VAL
1	A	1048	VAL
1	A	1090	VAL
1	A	1109	LEU
1	A	1111	ILE
1	A	1163	THR
1	A	1167	ASP
1	A	1168	LYS
1	B	35	VAL
1	B	81	VAL
1	B	90	GLN
1	B	129	VAL
1	B	156	ILE
1	B	258	ARG
1	B	279	GLU
1	B	310	PHE
1	B	335	LEU
1	B	373	SER
1	B	383	ASN
1	B	435	LEU
1	B	474	VAL
1	B	478	THR
1	B	603	VAL
1	B	688	VAL
1	B	753	LEU
1	B	755	PHE
1	B	863	ILE
1	B	886	LEU
1	B	906	LEU
1	B	908	ARG
1	B	930	LYS
1	B	944	MET
1	B	966	THR
1	B	967	PHE
1	B	972	LEU
1	B	1022	LEU
1	B	1037	VAL

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Mol	Chain	Res	Type
1	B	1046	ILE
1	B	1048	VAL
1	B	1090	VAL
1	B	1109	LEU
1	B	1111	ILE
1	B	1163	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	514	HIS
1	A	515	GLN
1	A	717	ASN
1	A	838	ASN
1	A	852	GLN
1	A	942	GLN
1	A	1149	ASN
1	B	347	ASN
1	B	392	ASN
1	B	394	HIS
1	B	404	GLN
1	B	514	HIS
1	B	515	GLN
1	B	838	ASN
1	B	1108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1188/1282 (92%)	-0.09	16 (1%)	75 53	84, 141, 236, 375	0
1	B	1180/1282 (92%)	-0.15	21 (1%)	67 46	86, 152, 247, 420	0
All	All	2368/2564 (92%)	-0.12	37 (1%)	70 48	84, 146, 241, 420	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	GLY	5.1
1	A	423	GLY	4.5
1	B	1060	GLN	4.2
1	A	871	GLU	4.2
1	B	598	ASP	4.1
1	A	1123	ILE	3.9
1	A	443	LEU	3.8
1	B	1021	GLY	3.8
1	B	974	PHE	3.4
1	B	1212	GLU	3.3
1	B	184	ASP	3.3
1	A	1244	ASN	3.2
1	A	987	VAL	3.2
1	B	950	ALA	3.2
1	A	1124	ALA	2.8
1	B	1020	GLN	2.7
1	B	601	VAL	2.7
1	A	1011	THR	2.6
1	A	184	ASP	2.6
1	B	1024	PRO	2.5
1	A	1127	ILE	2.5
1	B	768	LEU	2.5
1	B	205	THR	2.4
1	B	1061	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	852	GLN	2.3
1	A	133	CYS	2.3
1	A	1063	ALA	2.3
1	A	1223	CYS	2.3
1	B	978	VAL	2.3
1	A	1045	SER	2.1
1	B	179	ASN	2.1
1	A	964	LEU	2.1
1	B	1233	ILE	2.0
1	B	133	CYS	2.0
1	B	990	PHE	2.0
1	A	99	MET	2.0
1	B	1228	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	A	1307	1/1	0.58	0.31	138,138,138,138	1
2	HG	B	1303	1/1	0.62	0.10	198,198,198,198	1
2	HG	A	1302	1/1	0.71	0.34	71,71,71,71	1
2	HG	A	1306	1/1	0.81	0.18	96,96,96,96	1
2	HG	B	1305	1/1	0.83	0.38	46,46,46,46	1
2	HG	B	1302	1/1	0.89	0.14	189,189,189,189	1
2	HG	A	1305	1/1	0.90	0.32	65,65,65,65	1
2	HG	A	1303	1/1	0.92	0.27	102,102,102,102	1
2	HG	B	1301	1/1	0.95	0.17	129,129,129,129	1
2	HG	B	1306	1/1	0.96	0.21	71,71,71,71	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	B	1304	1/1	0.97	0.16	107,107,107,107	1
2	HG	A	1301	1/1	0.97	0.12	164,164,164,164	1
2	HG	A	1304	1/1	0.97	0.28	38,38,38,38	1

6.5 Other polymers [i](#)

There are no such residues in this entry.